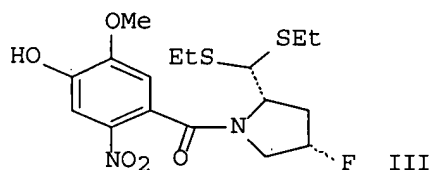
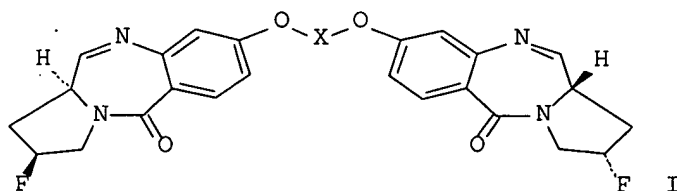


L5 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2005:1078234 CAPLUS Full-text
 DN 143:347210
 TI A preparation of fluoropyrrolobenzodiazepine dimers, useful as antitumor agents
 IN Kamal, Ahmed; Reddy, Peram Surakattula Murali Mohan; Reddy, Depatla Rajashekhar
 PA Council of Scientific and Industrial Research, India
 SO U.S. Pat. Appl. Publ., 13 pp.
 CODEN: USXXCO
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2005222131	A1	20051006	US 2004-812840	20040330
PRAI	US 2004-812840		20040330		

GI



AB The invention relates to a preparation of fluoropyrrolobenzodiazepine dimers of formula I [wherein: X is (CH₂)₃₋₁₀], useful as antitumor agents. For instance, fluoropyrrolobenzodiazepine dimer II (I, X = (CH₂)₄; logGI₅₀ = -5.21, logTGI₅₀ = -4.75) was prepared from diethylthioacetal derivative III via 3 steps.

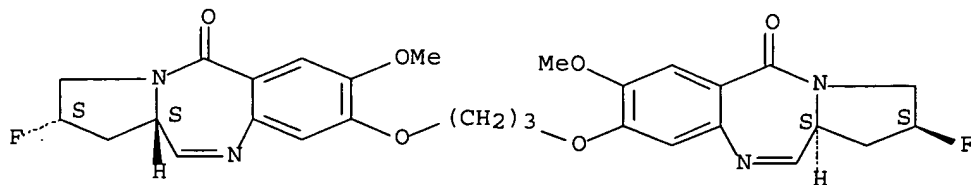
IT 717920-82-6P 717920-83-7P 717920-84-8P
 858639-17-5P 858639-19-7P 858639-21-1P
 858639-23-3P 858639-25-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of fluoropyrrolobenzodiazepine dimers useful as antitumor agents)

RN 717920-82-6 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,3-propanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

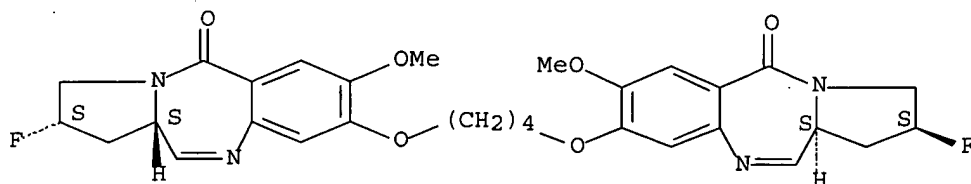


RN 717920-83-7 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,4-butanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-,

(2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

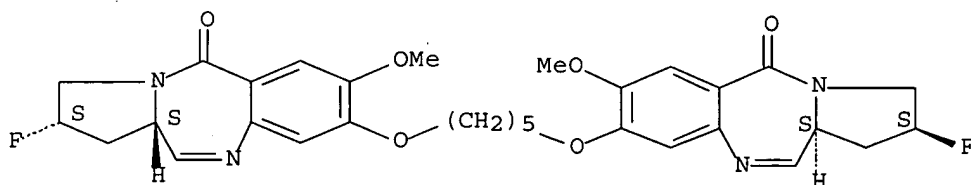
Absolute stereochemistry.



RN 717920-84-8 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,5-pentanediy]bis(oxy)bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

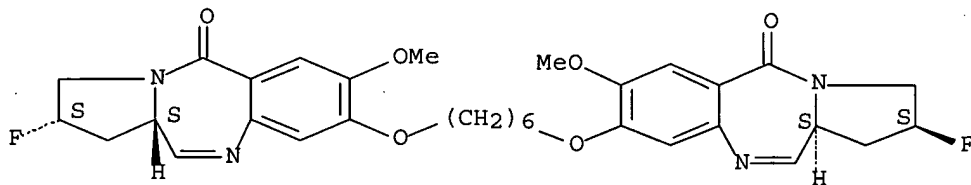
Absolute stereochemistry.



RN 858639-17-5 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,6-hexanediy]bis(oxy)bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

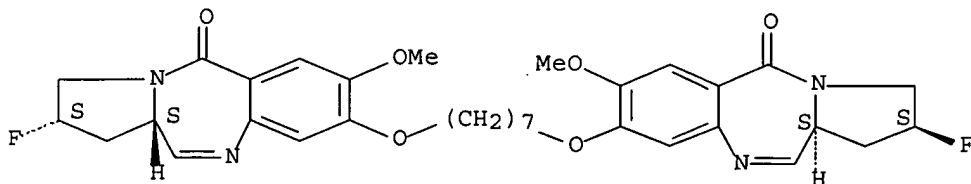
Absolute stereochemistry.



RN 858639-19-7 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,7-heptanediy]bis(oxy)bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

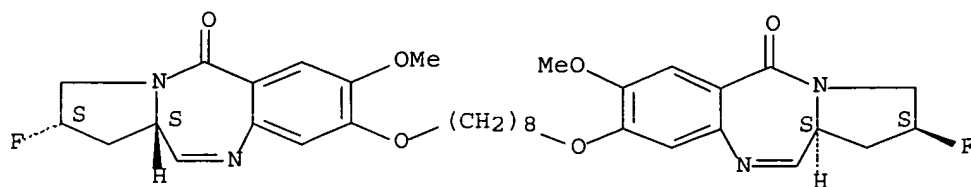
Absolute stereochemistry.



RN 858639-21-1 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,8-octanediy]bis(oxy)bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

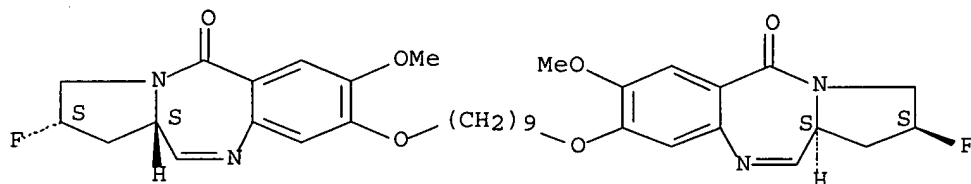
Absolute stereochemistry.



RN 858639-23-3 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,9-nonanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

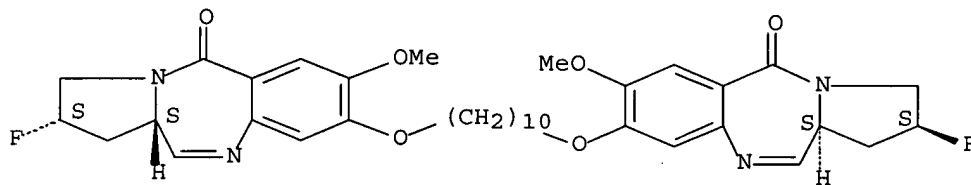
Absolute stereochemistry.



RN 858639-25-5 CAPLUS

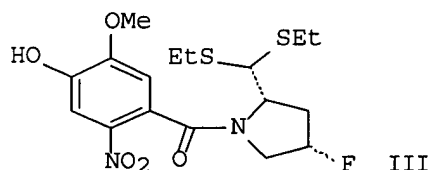
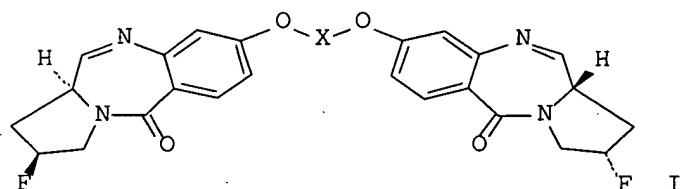
CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,10-decanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2005:612296 CAPLUS Full-text
 DN 143:133404
 TI A preparation of fluoropyrrolobenzodiazepine dimers, useful as antitumor agents
 IN Kamal, Ahmed; Reddy, Peram Surakattula Murali Mohan; Reddy, Depatla Rajasekhar
 PA Council of Scientific and Industrial Research, India
 SO PCT Int. Appl., 28 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005063758	A1	20050714	WO 2003-IN448	20031231
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRAI	WO 2003-IN448		20031231		
OS	CASREACT 143:133404				
GI					



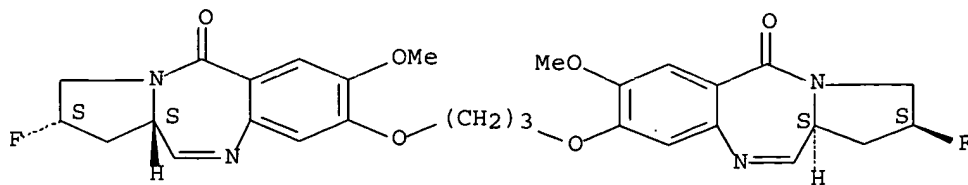
AB The invention relates to a preparation of fluoropyrrolobenzodiazepine dimers of formula I [wherein: X is (CH₂)₃₋₁₀], useful as antitumor agents. For instance, fluoropyrrolobenzodiazepine dimer II (I, X = CH₂)₄; (logGI50 = -5.21, logTGI50 = -4.75) was prepared from diethylthioacetal derivative III via 3 steps.

IT 717920-82-6P 717920-83-7P 717920-84-8P
 858639-17-5P 858639-19-7P 858639-21-1P
 858639-23-3P 858639-25-5P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of fluoropyrrolobenzodiazepine dimers useful as antitumor agents)

RN 717920-82-6 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,3-propanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS)- (9CI) (CA INDEX NAME)

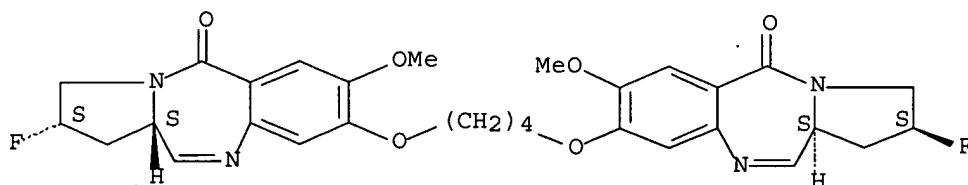
Absolute stereochemistry.



RN 717920-83-7 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,4-butanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

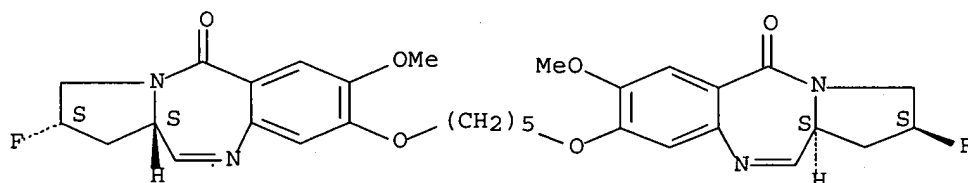
Absolute stereochemistry.



RN 717920-84-8 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,5-pentanediybis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

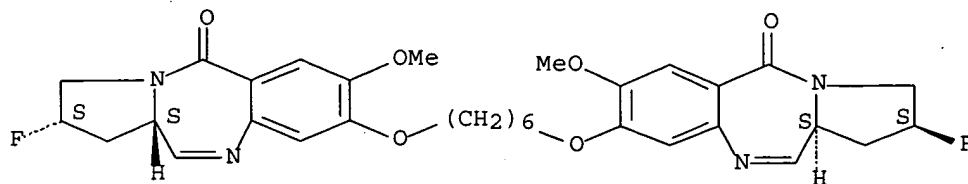
Absolute stereochemistry.



RN 858639-17-5 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,6-hexanediybis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

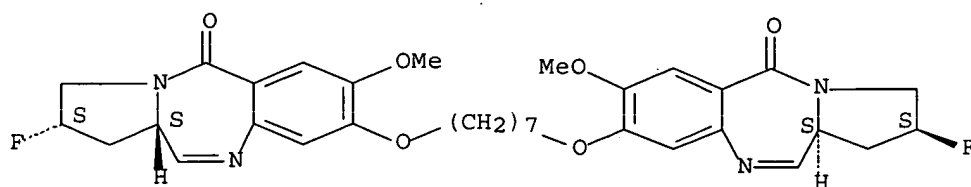
Absolute stereochemistry.



RN 858639-19-7 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,7-heptanediybis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

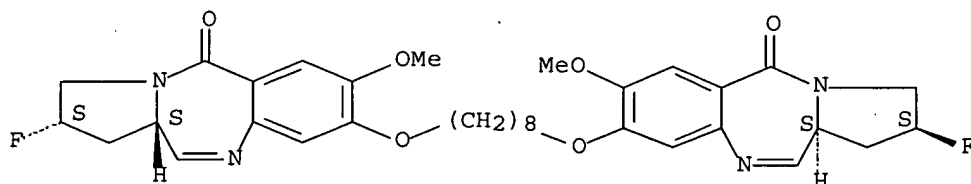
Absolute stereochemistry.



RN 858639-21-1 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,8-octanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

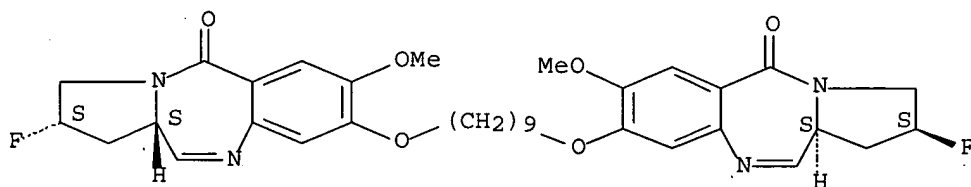
Absolute stereochemistry.



RN 858639-23-3 CAPLUS

CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,9-nonanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

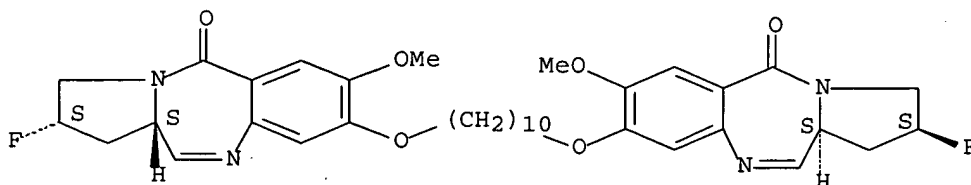
Absolute stereochemistry.



RN 858639-25-5 CAPLUS

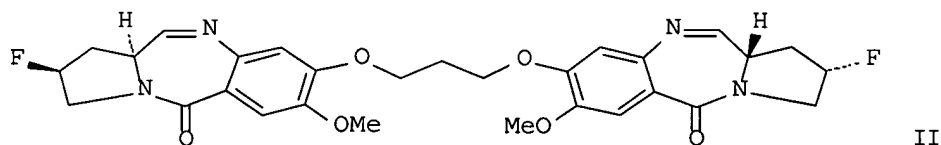
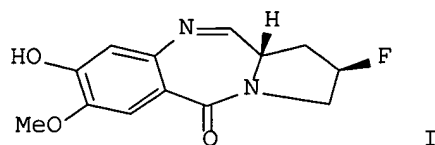
CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,10-decanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



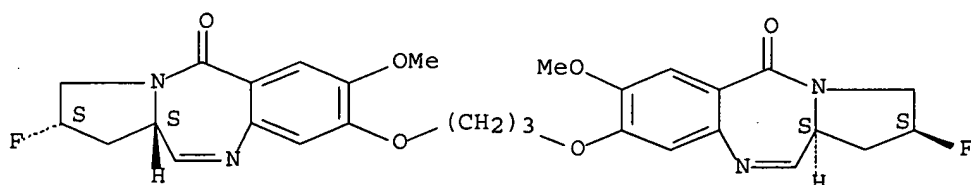
RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2004:346285 CAPLUS Full-text
 DN 141:106440
 TI The effect of C2-fluoro group on the biological activity of DC-81 and its dimers
 AU Kamal, Ahmed; Reddy, P. S. M. M.; Reddy, D. Rajasekhara
 CS Division of Organic Chemistry, Biotransformation Laboratory, Indian Institute of Chemical Technology, Hyderabad, 500007, India
 SO Bioorganic & Medicinal Chemistry Letters (2004), 14(10), 2669-2672
 CODEN: BMCLE8; ISSN: 0960-894X
 PB Elsevier Science B.V.
 DT Journal
 LA English
 OS CASREACT 141:106440
 GI



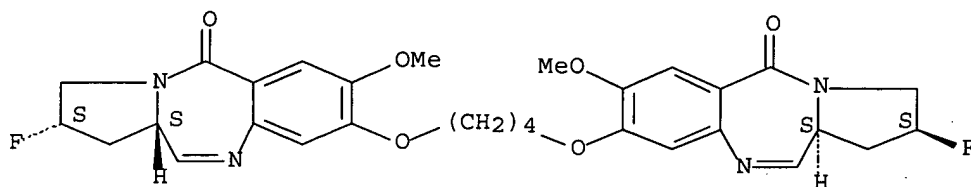
AB C2-Fluoro substituted pyrrolobenzodiazepines were synthesized that exhibit potential anticancer activity in a number of human tumor cell lines. These C2-fluoro substituted PBDs also exhibit significant DNA-binding ability. Example compds. included (2R,11aS)-2-Fluoro-1,2,3,11a-tetrahydro-8-hydroxy-7-methoxy-5H-pyrrolo[2,1-c][1,4]benzodiazepin-5-one (I) and a dimer (II).
 IT 717920-82-6P 717920-83-7P 717920-84-8P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (preparation of (fluoro)tetrahydro(hydroxy)pyrrolo[2,1-c][1,4]benzodiazepin-5-one derivs. and dimers and study of their anticancer activity)
 RN 717920-82-6 CAPLUS
 CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,3-propanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



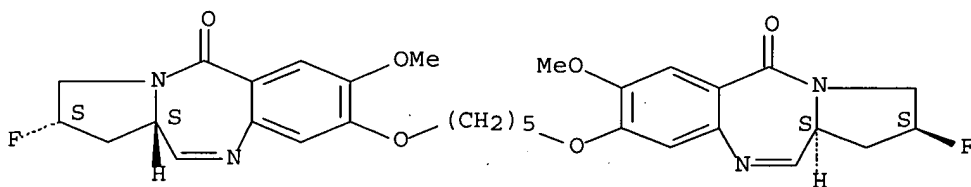
RN 717920-83-7 CAPLUS
 CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,4-butanediylbis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 717920-84-8 CAPLUS
 CN 5H-Pyrrolo[2,1-c][1,4]benzodiazepin-5-one, 8,8'-[1,5-pentanediyibis(oxy)]bis[2-fluoro-1,2,3,11a-tetrahydro-7-methoxy-, (2S,2'S,11aS,11'aS) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

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 L4 8 S L2 FUL

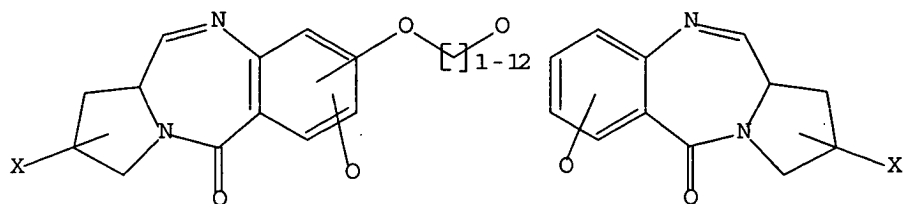
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L5 3 S L4

=> d 12; d his

L2 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.
 L2 QUE ABB=ON PLU=ON L1

(FILE 'HOME' ENTERED AT 09:33:29 ON 27 JAN 2006)

FILE 'REGISTRY' ENTERED AT 09:34:02 ON 27 JAN 2006

L1 STRUCTURE UPLOADED
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 L4 8 S L2 FUL

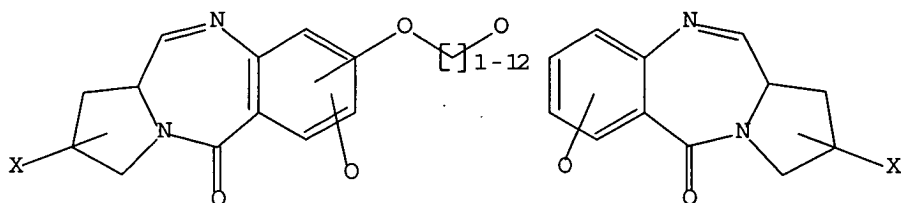
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L5 3 S L4

=> d l2; d his; log y

L2 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.
 L2 QUE ABB=ON PLU=ON L1

(FILE 'HOME' ENTERED AT 09:33:29 ON 27 JAN 2006)

FILE 'REGISTRY' ENTERED AT 09:34:02 ON 27 JAN 2006

L1 STRUCTURE UPLOADED
 L2 QUE L1
 L3 1 S L2
 L4 8 S L2 FUL

FILE 'CAPLUS' ENTERED AT 09:34:28 ON 27 JAN 2006

L5

3 S L4

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	15.79	182.94
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-2.25	-2.25

STN INTERNATIONAL LOGOFF AT 09:35:03 ON 27 JAN 2006